

Continuous optimal ensembles I: A geometrical characterization of robustly separable quantum states

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Abstract

A geometrical characterization of robustly separable (that is, remaining separable under sufficiently small variations) mixed states of a bipartite quantum system is given. It is shown that the density matrix of any such state can be represented as a normal vector to a hypersurface in the Euclidean space of all self-adjoint operators in the state space of the whole system. The expression for this hypersurface is provided.

1 Introduction

Entanglement turned out to be a crucial resource for quantum computation. It plays a central rôle in quantum communication and quantum computation. A considerable effort is being put into quantifying quantum entanglement.

It seems natural to focus the efforts on quantifying entanglement itself, that is, describing the *impossibility* to prepare a state by means of LOCC (local operations and classical communications). One may, although, go another way around and try to quantify *separability* rather than entanglement: this turned out to be applicable for building combinatorial entanglement patterns for multipartite quantum systems [4].

In this paper I dwell on the case of bipartite quantum systems. A state of such system is called SEPARABLE if it can be prepared by LOCC. In terms

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of density matrices that means that \mathbf{p} , its density matrix, can be represented as a mixture of pure product states. According to Carathéodory theorem, the number of this states can be reduced to n^4 where n is the dimension of the state of a single particle.

The idea to replace finite sums of projectors by continuous distributions on the set of unit vectors is put forward making it possible to provide a geometrical characterization of separable mixed states of a bipartite quantum system. To consistently describe the result presented in this paper recall some necessary definitions.

Basics. A density matrix \mathbf{p} in the product space \mathfrak{B} is called FACTORIZABLE if it is a tensor product of density matrices, $\mathbf{p} = \rho \otimes \rho'$. If \mathbf{p} is a convex combination of factorizable operators, it is said to be SEPARABLE

$$\mathbf{p} = \sum_{\alpha} p_{\alpha} \rho_{\alpha} \otimes \rho'_{\alpha} \quad (1)$$

A crucial feature of quantum mechanics, the phenomenon of quantum entanglement, stems from the fact that there exist density operators in the product space which are NOT separable, they are called ENTANGLED. A density operator \mathbf{p} is called ROBUSTLY SEPARABLE if it has a neighborhood U in \mathcal{L} such that all operators $\rho' \in U$ are separable.

A brief account. In the Euclidean space \mathfrak{L} of self-adjoint operators acting in the tensor product space $\mathfrak{B} = \mathcal{H} \otimes \mathcal{H}'$ we define a real-valued, positive functional $\mathcal{K} : \mathfrak{L} \rightarrow \mathbb{R}_+$ as follows

$$\mathcal{K}(X) = \iint e^{\langle \phi \phi' | X | \phi \phi' \rangle} d\mathbf{S}_n d\mathbf{S}'_n$$

where the integration is taken over the torus—the Cartesian product of unit spheres in $\mathcal{H}, \mathcal{H}'$, respectively, and consider the hypersurface $\mathcal{K} \subset \mathfrak{L}$

$$\mathcal{K} = \{X \in \mathfrak{L} \mid \mathcal{K}(X) = 1\}$$

Then

- all robustly separable density operators in \mathcal{H} are in 1–1 correspondence with the points of \mathcal{K}

- the density matrix associated with a point $X \in \mathcal{K}$ is the normal vector to \mathcal{K} at point X .

2 Continuous optimal ensembles

To make the account self-consistent, begin with necessary definitions. A DENSITY OPERATOR is a non-negative self-adjoint operator whose trace equals to 1. In particular, for any unit vector $|\phi\rangle$ the one-dimensional projector $|\phi\rangle\langle\phi|$ is a density matrix. Note that for any set of density operators ρ_α the convex combination $\sum_\alpha \rho_\alpha$ is always a density operator.

The set of all self-adjoint operators in $\mathcal{H} = \mathbb{C}^n$ has a natural structure of a real space \mathbb{R}^{2n} , in which the set of all density matrices is a hypersurface, which is the zero surface $T = 0$ of the affine functional $T = \text{Tr } X - 1$.

In this paper a geometrical characterization of separable bipartite density operators is provided. It is based on the notion of continuous ensembles. Generalizing the fact that any convex combination of density operators is again a density operator, we represent density operators as probability distributions on the unit sphere in the state space \mathcal{H} of the system. Let us pass to a more detailed account of this issue beginning with the case of a single quantum system.

Let $\mathcal{H} = \mathbb{C}^n$ be a n -dimensional Hermitian space, let ρ be a density matrix in \mathcal{H} . We would like to represent the state whose density operator is ρ by an ensemble of pure states. We would like this ensemble to be continuous with the probability density expressed by a function $\mu(\phi)$ where ϕ ranges over all unit vectors in \mathcal{H} .

Technical remark. Pure states form a projective space rather than the unit sphere in \mathcal{H} . On the other hand, one may integrate over any probabilistic space. Usually distributions of pure states over the spectrum of observables are studied, sometimes probability distributions on the projective spaces are considered [2]. In this paper for technical reasons I prefer to represent ensembles of pure states by measures on unit vectors in \mathcal{H} . I use the Umegaki measure on $\mathbb{C}B_n$ — the uniform measure with respect to the action of $U(n)$ normalized so that $\int_{\mathbb{C}B_n} d\mathbf{S}_n = 1$.

2.1 Effective definition

The density operator of a continuous ensemble associated with the measure $\mu(\phi)$ on the set $\mathbb{C}B_n$ of unit vectors in \mathcal{H} is calculated as the following (matrix) integral

$$\rho = \int_{\phi \in \mathbb{C}B_n} \mu(\phi) |\phi\rangle\langle\phi| d\mathbf{S}_n \quad (2)$$

where $|\phi\rangle\langle\phi|$ is the projector onto the vector $|\phi\rangle$ and $d\mathbf{S}_n$ is the above mentioned normalized measure on $\mathbb{C}B_n$:

$$\int_{\phi \in \mathbb{C}B_n} d\mathbf{S}_n = 1 \quad (3)$$

Effectively, the operator integral ρ in (2) can be calculated by its matrix elements. In any fixed basis $\{|\mathbf{e}_i\rangle\}$ in \mathcal{H} , each its matrix element $\rho_{ij} = \langle \mathbf{e}_i | \rho | \mathbf{e}_j \rangle$ is the following numerical integral:

$$\rho_{ij} = \langle \mathbf{e}_i | \rho | \mathbf{e}_j \rangle = \int_{\phi \in \mathbb{C}B_n} \mu(\phi) \langle \mathbf{e}_i | \phi \rangle \langle \phi | \mathbf{e}_j \rangle d\mathbf{S}_n \quad (4)$$

2.2 Optimal ensembles

We need to solve the following variational problem. Given a functional Q on $L^1(\mathbb{C}B_n)$ and given a density matrix ρ in \mathcal{H} , find the distribution μ on the set $\mathbb{C}B_n$ of unit vectors in \mathcal{H} such that

$$\begin{cases} \int_{\phi \in \mathbb{C}B_n} \mu(\phi) |\phi\rangle\langle\phi| d\mathbf{S}_n = \rho \\ Q(\mu) \rightarrow \text{extr} \end{cases} \quad (5)$$

We shall consider functionals Q of the form

$$Q(\mu) = \int_{\phi \in \mathbb{C}B_n} q(\mu(\phi)) d\mathbf{S}_n \quad (6)$$

then, according to (4), the variational problem (5) reads

$$\begin{cases} \int_{\phi \in \mathbb{C}B_n} \mu(\phi) \langle \mathbf{e}_i | \phi \rangle \langle \phi | \mathbf{e}_j \rangle d\mathbf{S}_n = \rho_{ij} \\ \int_{\phi \in \mathbb{C}B_n} q(\mu(\phi)) d\mathbf{S}_n \rightarrow \text{extr} \end{cases}$$

Solving this variational problem by introducing Lagrangian multiples X_{ij} we get

$$q'(\mu(\phi)) - \sum_{ij} X_{ij} \langle \mathbf{e}_i | \phi \rangle \langle \phi | \mathbf{e}_j \rangle = 0 \quad (7)$$

Combining the Lagrange multiples into the operator $X = \sum_{ij} X_{ij} |\mathbf{e}_j\rangle\langle\mathbf{e}_i|$ turns the equation (7) to $q'(\mu(\phi)) = \langle \phi | X | \phi \rangle$. Then, denoting by f the inverse of q' we write (7) as

$$\mu(\phi) = f(\langle \phi | X | \phi \rangle) \quad (8)$$

and the problem reduces to finding μ from the condition

$$\int_{\phi \in \mathbb{C}B_n} \mu(\phi) |\phi\rangle\langle\phi| d\mathbf{S}_n = \rho \quad (9)$$

which according to (8) and (4) can be written as

$$\langle \mathbf{e}_i | \rho | \mathbf{e}_j \rangle = \int_{\phi \in \mathbb{C}B_n} f(\langle \phi | X | \phi \rangle) |\phi\rangle\langle\phi| d\mathbf{S}_n \quad (10)$$

It follows from (7) that the coefficients X_{ik} can be chosen so that $X_{ik} = \bar{X}_{ki}$. That means that the problem of finding the optimal ensemble reduces to that of finding the coefficients of a self-adjoint operator, that is, to finding n^2 numbers from n^2 equations.

2.3 Geometrical interpretation

The equation (10) can be given a direct geometrical meaning. Let $\mathcal{L} \simeq \mathbb{R}^{n^2}$ be the space of all self-adjoint operators in \mathcal{H} . Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be a differentiable function. Consider the real valued functional $F : \mathcal{L} \rightarrow \mathbb{R}$ defined as

$$F(X) = \int_{\phi \in \mathbb{C}B_n} f(\langle \phi | X | \phi \rangle) d\mathbf{S}_n \quad (11)$$

which is well-defined as the set $\mathbb{C}B_n$ is compact. Fix a basis $\{\mathbf{e}_k\}$ in \mathcal{H} , then any $X \in \mathcal{L}$ is defined by its matrix elements $X_{ik} = \langle \mathbf{e}_i | X | \mathbf{e}_k \rangle$, so $\langle \phi | X | \phi \rangle = \sum_{ik} X_{ik} \langle \phi | \mathbf{e}_i \rangle \langle \mathbf{e}_k | \phi \rangle$. Then the expression (11) can be treated as an integral depending on the set of parameters $\{X_{ik}\}$. We may consider the derivatives of $F(X)$ with respect to these variables, calculate them

$$\begin{aligned}
\frac{\partial}{\partial X_{ik}} F(X) &= \int_{\phi \in \mathbb{C}B_n} \frac{\partial}{\partial X_{ik}} \left(f(\langle \phi | X | \phi \rangle) \right) d\mathbf{S}_n = \\
&= \int_{\phi \in \mathbb{C}B_n} f'(\langle \phi | X | \phi \rangle) \langle \phi | \mathbf{e}_i \rangle \langle \mathbf{e}_k | \phi \rangle d\mathbf{S}_n = \\
&= \langle \mathbf{e}_k | \int_{\phi \in \mathbb{C}B_n} f'(\langle \phi | X | \phi \rangle) |\phi\rangle\langle\phi| d\mathbf{S}_n | \mathbf{e}_i \rangle
\end{aligned} \tag{12}$$

So, the gradient of the functional F is the operator which can be symbolically written as

$$\nabla F = \int_{\phi \in \mathbb{C}B_n} f'(\langle \phi | X | \phi \rangle) |\phi\rangle\langle\phi| d\mathbf{S}_n \tag{13}$$

and effectively calculated using (12).

2.4 Optimal entropy ensembles

Let us specify the form of the optimality functional in (6) assuming it to be the differential entropy of the appropriate distribution:

$$q(\mu) = -\mu \ln \mu \tag{14}$$

then $q' = -(1 + \ln \mu)$ and we have the following f for (10)

$$f(x) = e^{-(1+x)}$$

Introduce, as in (11), the functional $\mathcal{K} : \mathcal{L} \rightarrow \mathbb{R}$ on the set of all self-adjoint operators in \mathcal{H} (the minus sign and the unit summand are omitted here being a matter of renormalization):

$$\mathcal{K}(X) = \int_{\phi \in \mathbb{C}B_n} e^{\langle \phi | X | \phi \rangle} d\mathbf{S}_n \tag{15}$$

Note that $\rho(X) = \int_{\phi \in \mathbb{C}B_n} e^{\langle \phi | X | \phi \rangle} |\phi\rangle\langle\phi| d\mathbf{S}_n$ is always a positive operator, then

$$\mathcal{K}(X) = \text{Tr} \int_{\phi \in \mathbb{C}B_n} e^{\langle \phi | X | \phi \rangle} |\phi\rangle\langle\phi| d\mathbf{S}_n = 1$$

is a condition which defines a full-range density matrix $\rho(X)$ in \mathcal{H} . On the other hand, the condition $\mathcal{K}(X) = 1$ defines a hypersurface in the Euclidean space \mathcal{L} . Together with the fact that $(e^x)' = e^x$ and (13) we come to the following

Statement. Any full-range density matrix in ρ is associated with a point on the hypersurface $\mathcal{K}(X) = 1$ and the entries of ρ are calculated as the components of the gradient:

$$\rho = \nabla \mathcal{K} \quad (16)$$

2.5 The existence

Why optimal entropy ensembles do exist for all full-range density matrices? First note that for any full-range density matrix $\rho = \sum p_k |\mathbf{e}_k\rangle\langle\mathbf{e}_k|$ there are infinitely many continuous ensembles (=probability measures on $\mathbb{C}B_n$ in our setting) associated with it. An example of such distribution is $\rho = \sum p_k |\mathbf{e}_k\rangle\langle\mathbf{e}_k| = \int \mu(\phi) |\phi\rangle\langle\phi| d\mathbf{S}_n$ with

$$\mu(\phi) = \frac{((L+1)n)!}{L n! (L n)!} \sum_{k=1}^n \left(p_k - \frac{1}{L(n+1)} \right) |\langle \mathbf{e}_k | \phi \rangle|^{2Ln} \quad (17)$$

as it follows from [5]. Here L is a parameter, such that $L > \frac{1}{p_0(n+1)}$ where $p_0 > 0$ is the smallest eigenvalue of ρ . Any probabilistic density μ whose support is $\mathbb{C}B_n$ is a point in the interior of the simplex of all probabilistic measures on $\mathbb{C}B_n$. For each probabilistic measure on $\mathbb{C}B_n$ its differential entropy can be calculated. The differential entropy is, in turn, a concave function in the affine space of probability distributions. Therefore if we have an affine subset of of probability measure on $\mathbb{C}B_n$, the differential entropy takes its maximal value in the interior of the simplex of probability measures. Now return to the condition in (5)—we see that it is affine. Therefore, if we know that there exist at least one continuous ensemble representing ρ (but

we know that as mentioned above), that means that there exist a maximal entropy ensemble representing X , hence it has the representation (16).

3 Bipartite systems

Consider two finite-dimensional quantum systems whose state spaces are $\mathcal{H}, \mathcal{H}'$. The state space of the composite system is the tensor product $\mathfrak{B} = \mathcal{H} \otimes \mathcal{H}'$. Denote by $\mathfrak{L} = \mathcal{L} \otimes \mathcal{L}$ the space of all self-adjoint operators in \mathfrak{B} .

3.1 Continuous ensembles in bipartite case

Let \mathbf{p} be a robustly separable density matrix in the product space $\mathcal{H} \otimes \mathcal{H}'$. Then it can be represented (in infinitely many ways) as a continuous ensemble of pure product states. Carrying out exactly the same reasoning as in section 2.5 we conclude that among those continuous ensembles there exists one having the least differential entropy, this will be the ensemble we are interested in. Like in section 2.4, formulate the variational problem. Let \mathbf{p} be a density operator in a tensor product space $\mathfrak{B} = \mathcal{H} \otimes \mathcal{H}'$. The task is to find a probability density $\mu(\phi\phi')$ defined on the Cartesian product $\mathfrak{T} = \mathbb{C}B_n \times \mathbb{C}B_n$ of the unit spheres in $\mathcal{H}, \mathcal{H}'$, respectively.

$$\begin{cases} \int_{\phi\phi' \in \mathfrak{T}} \mu(\phi\phi') |\phi\phi'\rangle\langle\phi\phi'| d\mathbf{S}_n d\mathbf{S}'_n = \mathbf{p} \\ Q(\mu) \rightarrow \text{extr} \end{cases} \quad (18)$$

Proceeding exactly in the same way as with single particle, we get the following representation:

$$\mathbf{p} = \int_{\phi\phi' \in \mathfrak{T}} e^{\langle\phi\phi'|X|\phi\phi'\rangle} |\phi\phi'\rangle\langle\phi\phi'| d\mathbf{S}_n d\mathbf{S}'_n \quad (19)$$

for some self-adjoint operator X in \mathcal{L} whose existence is guaranteed by the same reasons as in section 2.5. Why such X does not exist for entangled density operators? The reason is that the set of probability distributions among which $e^{\langle\phi\phi'|X|\phi\phi'\rangle}$ is optimal is simply void in the entangled case.

3.2 Geometrical characterization of robustly separable quantum states

Now we pass to the main result of this paper. Suppose we deal with a tensor product of two Hilbert spaces $\mathcal{H}, \mathcal{H}'$, each of dimension n . Consider the space \mathcal{L} of all self-adjoint linear operators in the tensor product $\mathfrak{B} = \mathcal{H} \otimes \mathcal{H}'$, being a Euclidean space of dimension n^4 . For any $X \in \mathcal{L}$ we can always calculate the integral

$$\mathcal{K}(X) = \int_{\phi\phi' \in \mathfrak{T}} e^{\langle \phi\phi' | X | \phi\phi' \rangle} d\mathbf{S}_n d\mathbf{S}'_n \quad (20)$$

which is always well-defined (as an integral of a bounded function over a compact set), positive (as the exponent is always positive) functional from \mathcal{L} to \mathbb{R}_+ . Consider the hypersurface \mathcal{K} in \mathcal{L} defined by the equation

$$\mathcal{K} = \{X \in \mathcal{L} \mid \mathcal{K}(X) = 1\}$$

In any point of \mathcal{L} the gradient $\nabla \mathcal{K}$ can be calculated. In particular, at any point X of \mathcal{K} the gradient $\nabla \mathcal{K}$ will be a normal vector to \mathcal{K} . The surface \mathcal{K} is something given once and forever, it depends only on the dimensionality of the state space. For any X such that $\mathcal{K}(X) = 1$, we can calculate the gradient $\mathbf{p}(X) = \nabla \mathcal{K}|_X$ at point X . Fix bases $\{\mathbf{e}_i\}, \{\mathbf{e}'_{i'}\}$, then $X = \sum_{ii' kk'} X_{ii' kk'} |ii'\rangle\langle kk'|$ and the expression (19) for the operator \mathbf{p} has the following form:

$$\mathbf{p}_{ii' kk'} = \nabla \mathcal{K} = \frac{\partial \mathcal{K}}{\partial X_{ii' kk'}} \quad (21)$$

Conversely, given a robustly separable bipartite density matrix \mathbf{p} , we know that it can be represented as a convex combination of product states: $\mathbf{p} = \sum p_\alpha \rho_\alpha \otimes \rho'_\alpha$. Each ρ_α can be, in turn, represented as a non-vanishing probability distribution (17). Then exactly the same reasoning as in section 2.5 can be carried out and there is a point X on the surface \mathcal{K} associated with \mathbf{p} . So, together with (21), we have the main result:

$$\{\text{robustly separable states}\} \leftrightarrow \{\text{the points of } \mathcal{K}\} \quad (22)$$

Summary

A geometrical interpretation of robustly separable density operators of a bipartite quantum system with the state space $\mathfrak{B} = \mathcal{H} \otimes \mathcal{H}'$ is provided. They are represented as normal vectors to the hypersurface \mathcal{K} in the (Euclidean) space \mathfrak{L} of self-adjoint operators in \mathfrak{B} defined by the following equation:

$$\mathcal{K} = \left\{ X \left| \int_{\phi\phi' \in \mathfrak{T}} e^{\langle \phi\phi' | X | \phi\phi' \rangle} d\mathbf{S}_n d\mathbf{S}'_n = 1 \right. \right\} \quad (23)$$

where the integration is performed over the set of all unit product vectors $|\phi\phi'\rangle \in \mathfrak{B}$. Each point $X \in \mathcal{K}$ is a self-adjoint operator, the parameter of the probability distribution on the set of unit vectors which gives a density operator \mathbf{p} . Furthermore, the normal vector to \mathcal{K} at point X is \mathbf{p} itself:

$$\mathbf{p} = \nabla \mathcal{K}|_X = \int_{\phi\phi' \in \mathfrak{T}} e^{\langle \phi\phi' | X | \phi\phi' \rangle} |\phi\phi'\rangle \langle \phi\phi'| d\mathbf{S}_n d\mathbf{S}'_n \quad (24)$$

The final remark. Given a density matrix \mathbf{p} in \mathfrak{B} , a question arises if it is separable or not. When the dimension of at least one of spaces $\mathcal{H}, \mathcal{H}'$ is 2, this question was given an effective answer—the positive partial transpose (PPT) criterion due to Peres-Horodecki was suggested [1]. The criterion states that \mathbf{p} is separable if and only if its partial transpose \mathbf{p}^{T_2} remains non-negative matrix. In higher dimensions PPT is only a necessary condition for a state to be factorizable as there exist entangled density matrices whose partial transpose is positive.

Although a geometrical characterization of robustly separable density matrices is provided, it does not solve (directly, at least) the ‘inverse problem’. Nevertheless, the continuous ensemble method presented in this paper seems to be helpful for tackling the inverse problem as well. This issue is addressed in the next paper on continuous ensembles.

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